



JOURNAL OF  
APPLIED  
CRYSTALLOGRAPHY

**Volume 51 (2018)**

**Supporting information for article:**

**Correct interpretation of diffraction properties of quartz crystals for X-ray optics applications**

**Xian-Rong Huang, Thomas Gog, Jung-ho Kim, Elina Kasman, Ayman H. Said, Diego M. Casa, Michael Wiczorek, Marcelo G. Hönnicke and Lahsen Assoufid**

## Supplementary Information

**Table S1. Back-reflections  $\{hkl\}$  ( $\theta_B = 90^\circ$ ) of Si with  $E_{BR} < 16$  keV at room temperature 293.15 K**

$E_{BR}$ : Back reflection Bragg energy ( $\theta_B = 90^\circ$ ).

$\Delta E_{BW}$ : Darwin bandwidth (FWHM of the energy-dependent Darwin curve at  $\theta_B = 90^\circ$ ).

$R_{max}$ : Maximum reflectivity of the Darwin curve.

Each  $\{hkl\}$  reflection represents all the crystallographic equivalent reflections  $\pm h \pm k \pm l$ .

The reflection in red color (with grey background) has the same  $E$ ,  $\Delta E_{BW}$ ,  $R_{max}$ , and rocking curve width as the reflection in regular color above it. For example, reflection  $\{511\}$  is equivalent to reflection  $\{333\}$  in X-ray diffraction, although they are not equivalent in crystallography. Thus,  $\{511\}$  is not counted as a different reflection in the 48 reflections.

#	$h$	$k$	$l$	$E_{BR}$ (keV)	$\Delta E_{BW}$ (meV)	$R_{max}$
[1]	1	1	1	1.97704	204.006	0.403323
[2]	2	2	0	3.22849	170.377	0.728434
[3]	3	1	1	3.78575	107.875	0.666351
[4]	4	0	0	4.56578	112.77	0.796533
[5]	3	3	1	4.97544	72.0807	0.740011
[6]	4	2	2	5.59192	82.225	0.829377
[7]	3	3	3	5.93112	53.2459	0.775919
	5	1	1	5.93112	53.2459	0.775919
[8]	4	4	0	6.45699	63.1292	0.847206
[9]	5	3	1	6.75288	41.2678	0.795756
[10]	6	2	0	7.21913	50.0635	0.857513
[11]	5	3	3	7.48496	32.9661	0.807325
[12]	4	4	4	7.90816	40.6393	0.863627
[13]	5	5	1	8.15155	26.9208	0.814209
	7	1	1	8.15155	26.9208	0.814209
[14]	6	4	2	8.54179	33.6025	0.867205
[15]	5	5	3	8.76761	22.3763	0.81822
	7	3	1	8.76761	22.3763	0.81822
[16]	8	0	0	9.13156	28.2357	0.869301
[17]	7	3	3	9.34313	18.9086	0.820684
[18]	6	6	0	9.68548	24.3084	0.871604
	8	2	2	9.68548	24.3084	0.871604
[19]	5	5	5	9.88521	16.2781	0.822859
	7	5	1	9.88521	16.2781	0.822859
[20]	8	4	0	10.2094	20.4545	0.869315
[21]	7	5	3	10.3991	13.7126	0.819151
	9	1	1	10.3991	13.7126	0.819151
[22]	6	6	4	10.7077	17.5531	0.867596
[23]	9	3	1	10.8887	11.8165	0.816824
[24]	8	4	4	11.1838	15.2281	0.865734

[25]	9	3	3	keV 11.3572	meV 10.2838	0.81427
	7	7	1	11.3572	10.2838	0.81427
	7	5	5	11.3572	10.2838	0.81427
[26]	10	2	0	11.6405	13.3248	0.863707
	8	6	2	11.6405	13.3248	0.863707
[27]	9	5	1	11.8072	9.0223	0.811489
	7	7	3	11.8072	9.0223	0.811489
[28]	9	5	3	12.2406	7.97143	0.808481
[29]	10	4	2	12.5039	10.4211	0.859109
[30]	11	1	1	12.6592	7.08736	0.805304
	7	7	5	12.6592	7.08736	0.805304
[31]	8	8	0	12.914	9.30049	0.856647
[32]	11	3	1	13.0644	6.33718	0.802013
	9	7	1	13.0644	6.33718	0.802013
	9	5	5	13.0644	6.33718	0.802013
[33]	10	6	0	13.3114	8.34446	0.854104
	8	6	6	13.3114	8.34446	0.854104
[34]	11	3	3	13.4574	5.69551	0.79864
	9	7	3	13.4574	5.69551	0.79864
[35]	12	0	0	13.6973	7.52305	0.851509
	8	8	4	13.6973	7.52305	0.851509
[36]	11	5	1	13.8393	5.14291	0.795164
	7	7	7	13.8393	5.14291	0.795164
[37]	12	2	2	14.0727	6.81249	0.848851
	10	6	4	14.0727	6.81249	0.848851
[38]	11	5	3	14.2109	4.66396	0.791649
	9	7	5	14.2109	4.66396	0.791649
[39]	12	4	0	14.4383	6.19441	0.846158
[40]	9	9	1	14.573	4.24634	0.788141
[41]	10	8	2	14.7948	5.65323	0.84346
[42]	13	1	1	14.9263	3.88014	0.784535
	11	7	1	14.9263	3.88014	0.784535
	11	5	5	14.9263	3.88014	0.784535
	9	9	3	14.9263	3.88014	0.784535
[43]	12	4	4	15.143	5.1772	0.840708
[44]	13	3	1	15.2715	3.55725	0.780963
	11	7	3	15.2715	3.55725	0.780963
	9	7	7	15.2715	3.55725	0.780963
[45]	12	6	2	15.4833	4.75609	0.837958
[46]	13	3	3	15.609	3.27134	0.777337
	9	9	5	15.609	3.27134	0.777337
[47]	8	8	8	15.8163	4.38201	0.835197
[48]	13	5	1	15.9394	3.0169	0.773704
	11	7	5	15.9394	3.0169	0.773704

**Table S2**

**Complete list of back-reflections  $\{h_1 h_2 h_3 l\}$  ( $\theta_B = 90^\circ$ ) of left-handed  $\alpha$ -quartz with  $E_{BR} < 16$  keV and  $R_{\max} \geq 0.3$  at room temperature 293.15 K**

$E_{BR}$ : Back reflection Bragg energy ( $\theta_B = 90^\circ$ ).

$\Delta E_{BW}$ : Darwin bandwidth (FWHM of the Darwin curve as a function of  $E$  at  $\theta_B = 90^\circ$ ).

$R_{\max}$ : Maximum reflectivity of the Darwin curve.

$\Delta R_{\max} = R_{\max}(\bar{h}_1 \bar{h}_2 \bar{h}_3 \bar{L}) - R_{\max}(h_1 h_2 h_3 L)$  (anomalous scattering induced breakdown of Friedel's law)

- Each  $\{h_1 h_2 h_3 L\}$  reflection represents all the crystallographic equivalent reflections  $(h_1 h_2 h_3 L)$ ,  $(h_2 h_3 h_1 L)$ ,  $(h_3 h_1 h_2 L)$ ,  $(h_2 h_1 h_3 \bar{L})$ ,  $(h_3 h_2 h_1 \bar{L})$  and  $(h_1 h_3 h_2 \bar{L})$ , i.e., only one of the (six) equivalent reflections is listed in the table.
- For each reflection  $\{h_1 h_2 h_3 L\}$ , its opposite reflection  $\{\bar{h}_1 \bar{h}_2 \bar{h}_3 \bar{L}\}$  has exactly the same  $E$ ,  $\Delta E_{BW}$  and angular Darwin curve width, except that the  $R_{\max}$  can be different. Therefore, the  $\{\bar{h}_1 \bar{h}_2 \bar{h}_3 \bar{L}\}$  reflection is not listed in the table, but  $\Delta R_{\max} = R_{\max}(\bar{h}_1 \bar{h}_2 \bar{h}_3 \bar{L}) - R_{\max}(h_1 h_2 h_3 L)$  is presented with respect to each listed reflection  $\{h_1 h_2 h_3 L\}$ .
- $\{h_1 h_2 h_3 \bar{L}\}$  has exactly the same back reflection energy  $E$  as  $\{h_1 h_2 h_3 L\}$  (due to the same  $d$ -spacing), but the values of  $\Delta E_{BW}$  can be quite different. Such reflections are marked with gray background in the table. In the paper,  $\{h_2 h_1 h_3 L\}$  is used to represent such reflections, but note  $(h_2 h_1 h_3 L) = (h_1 h_2 h_3 \bar{L})$   $[= (h_1 h_3 h_2 L) = (h_3 h_2 h_1 L) = (h_3 h_1 h_2 \bar{L}) = (h_2 h_3 h_1 \bar{L})]$ .
- Geometrically, lattice planes  $\{70\bar{7} \pm L\}$  and  $\{8\bar{3}\bar{5} \pm L\}$  also have *exactly* the same  $d$ -spacing (corresponding to the same back-reflection energy but with different bandwidths), so do  $\{10\bar{1}\bar{9} \pm L\}$  and  $\{10\bar{5}\bar{6} \pm L\}$ . But these are special cases (in **Turquoise color** in the table) without generality.
- Our structure factor calculations follow the same algorithms as that used in the software package *XOP* (Del Rio, S. & Dejus, R. J. (2004). *Proc SPIE* **5536**, 171–174) using the equation

$$F_H = \sum_{n=1}^N \exp[-W_n(s)] (f_0(s) + f_1 + if_2) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_n) \quad (\text{Eq. S1})$$

where  $s = \sin \theta / \lambda = 1/(2d)$  and the atomic scattering factor is

$$f(s) = \sum_{j=1}^5 a_j \exp(-b_j s^2) + c. \quad (\text{Eq. S2})$$

Here we adopt the constants  $a_j$ ,  $b_j$  and  $c$  for each atom from *XOP*.  $f_1 + if_2$  is the (angle-independent) correction to the atomic scattering factor  $f_0$ , and the (energy-dependent) tabulated data of  $f_1 + if_2$  used in *XOP* are used in our program.  $\exp[-W_n(s)]$  is the Debye-Waller factor with

$$\begin{aligned} W(s) &= B(x)s^2, \\ x &= \frac{T_D}{T}, \\ B(x) &= \frac{6h^2}{mk_B T_D} \left( \frac{\Phi(x)}{x} + \frac{1}{4} \right), \\ \Phi(x) &= \frac{1}{x} \int_0^x \frac{y}{e^y - 1} dy. \end{aligned} \quad (\text{Eq. S3})$$

See R. W. James, *The Optical Principles of the Diffraction of X-Rays* (Woodbridge, Ox Bow Press, 1982) for details. The Debye temperatures we used here are derived from the data by Le Page, Y., Calvert, L. D. & Gabe E. J. (1980). *J. Phys. Chem. Solids* **41**, 721-725:  $T_D = 476.16^\circ\text{C}$  for the O atoms and  $516.88^\circ\text{C}$  for the Si atoms. In addition, we have also used the ABSORPTION program package from S. Brennan and P. L. Cowan [Rev. Sci. Instrum. **63**, 850 (1992)] to calculate the structure factors. This package does not use tabulated data but is purely based on quantum mechanics. Still it gives very similar structure factors very close to our program. We also used slightly different structures of quartz (including small variation of the Debye temperatures) reported in the literature to calculate the structure factors, and the results are nearly the same for strong reflections with  $R_{\max} \geq 0.3$ , with discrepancies less than 2%. For weak reflections (particularly the nearly forbidden reflections), the structure factors may change significantly, but such reflections are of no importance to the X-ray optics applications of quartz.

- The two-beam dynamical theory that takes into account the special back-reflection geometry [Shvyd'ko, Y. (2004). *X-ray Optics: High-Energy-Resolution Applications*, Berlin: Springer] is used for the Darwin curve computation.

#	#'	$h_1$	$h_2$	$h_3$	$L$	$E_{\text{BR}}$ (keV)	$\Delta E_{\text{BW}}$ (meV)	$R_{\max}$	$\Delta R_{\max}$
1	1	1	0	-1	0	1.45688	141.384	0.392882	0
2	2	1	0	-1	-1	1.85415	163.072	0.386132	9.68E-09
3	3	1	1	-2	0	2.52339	100.22	0.456775	-0.171658
4	4	1	0	-1	2	2.71735	83.1966	0.44121	1.57E-08
5	5	1	1	-2	-1	2.7718	54.731	0.381476	-0.275551
6	6	2	0	-2	0	2.91376	74.8688	0.504472	0
7	7	2	0	-2	1	3.13135	59.8852	0.372818	4.94E-09
8	8	2	-1	-1	2	3.41013	91.8723	0.633328	0.0155057
9	9	0	0	0	3	3.44069	34.5501	0.40236	3.33E-16
10	10	2	0	-2	2	3.7083	36.0581	0.365118	6.07E-09
11		2	0	-2	-2	3.7083	69.1202	0.603266	4.96E-09
12	11	1	0	-1	-3	3.73642	50.362	0.509734	-1.06E-08
13	12	3	-1	-2	1	4.02155	54.4685	0.602166	0.0620874
14		3	-1	-2	-1	4.02155	62.3779	0.657273	-0.0224994
15	13	2	-1	-1	3	4.26683	37.817	0.581664	-0.0778522
16	14	3	0	-3	0	4.37064	27.4953	0.443124	0
17	15	3	-1	-2	2	4.48542	34.5164	0.506965	0.100556
18		3	-1	-2	-2	4.48542	57.6329	0.724064	-0.0087164
19	16	2	0	-2	3	4.5087	91.2079	0.813286	-6.31E-10
20		2	0	-2	-3	4.5087	45.2692	0.675449	-1.17E-08
21	17	3	0	-3	-1	4.51861	81.2503	0.79445	-5.62E-10
22	18	1	0	-1	4	4.81337	54.4417	0.740823	-2.99E-09
23		1	0	-1	-4	4.81337	27.7624	0.578055	-8.26E-09
24	19	3	0	-3	2	4.93599	55.7269	0.770517	-3.58E-09
25		3	0	-3	-2	4.93599	38.4582	0.667645	1.35E-09
26	20	4	-2	-2	0	5.04678	49.0319	0.781987	-0.0535566

27	21	3	-1	-2	3	keV 5.1668	meV 44.9499	0.733073	0.0120458
28		3	-1	-2	-3	5.1668	22.3465	0.58898	-0.0887825
29	22	4	-2	-2	1	5.17546	26.5767	0.615929	-0.0279
30	23	2	-1	-1	4	5.23579	45.307	0.780407	-0.0532119
31	24	4	-1	-3	0	5.25286	47.9765	0.774517	-0.0156873
32	25	4	-1	-3	1	5.3766	19.0809	0.521655	0.0518259
33		4	-1	-3	-1	5.3766	34.0458	0.740745	-0.0780972
34	26	2	0	-2	4	5.4347	21.5758	0.576696	-1.60E-09
35	27	3	0	-3	3	5.56245	20.4629	0.580933	8.92E-09
36	28	4	-1	-3	2	5.73184	25.4487	0.630281	0.0878471
37		4	-1	-3	-2	5.73184	41.1983	0.802867	-0.0340218
38	29	4	0	-4	0	5.82752	28.7191	0.726914	0
39	30	1	0	-1	5	5.91666	24.2438	0.696294	-1.83E-09
40		1	0	-1	-5	5.91666	41.9989	0.804209	2.23E-09
41	31	4	0	-4	1	5.93931	38.3695	0.789286	-3.14E-10
42		4	0	-4	-1	5.93931	13.0467	0.495014	8.29E-10
43	32	3	-1	-2	4	5.99195	34.1795	0.789378	-0.0225838
44		3	-1	-2	-4	5.99195	7.69102	0.370073	-0.1435
45	33	4	-2	-2	3	6.10806	32.2223	0.764614	0.0269597
46	34	4	0	-4	2	6.26271	7.22456	0.322748	-1.06E-08
47		4	0	-4	-2	6.26271	19.4225	0.6721	1.80E-09
48	35	2	-1	-1	5	6.26513	26.6733	0.773969	-0.0476693
49	36	4	-1	-3	3	6.2794	14.0597	0.552664	0.0668879
50		4	-1	-3	-3	6.2794	16.0082	0.627016	-0.00378671
51	37	3	0	-3	4	6.33628	12.5094	0.545269	-5.69E-09
52		3	0	-3	-4	6.33628	17.104	0.665679	-7.87E-09
53	38	5	-2	-3	0	6.35039	23.1326	0.718594	0.00507281
54	39	2	0	-2	-5	6.43229	8.3678	0.411609	-9.93E-09
55	40	5	-2	-3	-1	6.45313	33.0242	0.821212	-0.0204277
56	41	5	-1	-4	0	6.67626	8.2494	0.446732	0.0314895
57	42	5	-2	-3	2	6.75196	18.6776	0.725526	0.00549791
58		5	-2	-3	-2	6.75196	6.28239	0.323808	0.0539436
59	43	4	0	-4	3	6.76745	31.1636	0.821832	-1.55E-09
60		4	0	-4	-3	6.76745	23.3201	0.771547	3.45E-09
61	44	5	-1	-4	1	6.77406	28.2013	0.79377	0.02382
62		5	-1	-4	-1	6.77406	11.3587	0.579501	-0.0037083
63	45	4	-2	-2	4	6.82026	18.3658	0.702342	0.0287696
64	46	0	0	0	6	6.88139	25.1908	0.797712	1.11E-16
65	47	3	-1	-2	5	6.90955	8.53235	0.558777	-0.113729
66		3	-1	-2	-5	6.90955	24.4749	0.798454	-0.0138037
67	48	4	-1	-3	4	6.97413	20.1865	0.743982	0.025799
68		4	-1	-3	-4	6.97413	12.2802	0.613254	0.0356176
69	49	1	0	-1	6	7.03392	16.0529	0.705568	1.18E-08
70	50	5	-1	-4	2	7.05932	12.2139	0.644639	-0.0175457

71		5	-1	-4	-2	keV 7.05932	meV 16.2996	0.739809	-0.0362804
72	51	3	0	-3	5	7.21019	15.0982	0.7224	1.09E-08
73		3	0	-3	-5	7.21019	5.95013	0.41115	4.97E-09
74	52	2	-1	-1	6	7.32946	11.5169	0.661115	-0.0171741
75	53	5	0	-5	-1	7.37413	11.345	0.674141	2.46E-10
76	54	4	0	-4	-4	7.4166	10.5361	0.634549	-8.23E-09
77	55	2	0	-2	6	7.47285	16.4886	0.762618	1.04E-08
78		2	0	-2	-6	7.47285	32.1867	0.866996	2.06E-09
79	56	5	-1	-4	3	7.51072	8.55551	0.603321	-0.0276027
80		5	-1	-4	-3	7.51072	24.968	0.831098	0.000862245
81	57	6	-3	-3	0	7.57017	20.9826	0.811878	-0.00389296
82	58	5	0	-5	2	7.63701	34.197	0.881444	1.87E-11
83	59	4	-2	-2	5	7.639	16.2473	0.752881	0.0196023
84	60	6	-3	-3	1	7.65656	15.761	0.742076	0.0330848
85	61	6	-2	-4	0	7.70908	21.5843	0.812839	0.0185143
86	62	4	-1	-3	5	7.77669	9.88058	0.667382	-0.0168323
87		4	-1	-3	-5	7.77669	13.71	0.719663	0.04446
88	63	6	-2	-4	1	7.79393	7.53016	0.588995	-0.00570568
89		6	-2	-4	-1	7.79393	11.1948	0.663999	0.0554561
90	64	5	-2	-3	4	7.83412	10.4273	0.681506	-0.0139447
91		5	-2	-3	-4	7.83412	26.7702	0.855099	0.0119167
92	65	3	-1	-2	6	7.88739	6.23815	0.573459	-0.0936647
93		3	-1	-2	-6	7.88739	15.7382	0.767182	0.0163058
94	66	6	-3	-3	2	7.91006	3.4745	0.349374	-0.0824127
95	67	6	-2	-4	2	8.0431	8.38341	0.664224	-0.0498919
96		6	-2	-4	-2	8.0431	17.4047	0.799835	0.0125573
97	68	5	0	-5	3	8.05611	3.925	0.366983	5.60E-09
98	69	5	-1	-4	4	8.10052	17.8769	0.821375	-0.0106709
99		5	-1	-4	-4	8.10052	4.43608	0.404224	0.0511952
100	70	6	-1	-5	0	8.11156	11.3918	0.706802	0.0465648
101	71	3	0	-3	-6	8.15205	10.1703	0.698381	-1.23E-08
102	72	1	0	-1	-7	8.1594	16.1981	0.802935	-5.05E-09
103	73	4	0	-4	5	8.17584	8.82761	0.664912	9.69E-09
104	74	6	-1	-5	1	8.19224	17.7016	0.815677	0.00443941
105		6	-1	-5	-1	8.19224	3.3059	0.346794	-0.0439723
106	75	6	-3	-3	3	8.3154	13.9342	0.784749	0.00304028
107	76	2	-1	-1	7	8.41551	13.552	0.77482	0.0217657
108	77	6	-1	-5	2	8.42965	5.38129	0.550198	-0.0146341
109		6	-1	-5	-2	8.42965	10.8983	0.747232	-0.00990889
110	78	6	-2	-4	3	8.44206	10.6281	0.781998	-0.0863147
111		6	-2	-4	-3	8.44206	12.1454	0.752686	0.0290183
112	79	4	-2	-2	6	8.53367	15.3142	0.813044	0.00663829
113	80	2	0	-2	7	8.54069	7.72763	0.662638	-1.02E-08
114		2	0	-2	-7	8.54069	6.73577	0.622992	-1.42E-08

115	81	5	-2	-3	5	keV 8.55639	meV 22.7178	0.868575	0.00753048
116		5	-2	-3	-5	8.55639	8.15061	0.68636	-0.0166025
117	82	5	0	-5	4	8.60863	3.12799	0.354176	-7.46E-09
118		5	0	-5	-4	8.60863	20.7813	0.864149	-1.47E-10
119	83	4	-1	-3	6	8.65713	10.011	0.747139	-0.0122888
120		4	-1	-3	-6	8.65713	8.65703	0.694458	0.026843
121	84	6	0	-6	0	8.74128	6.95272	0.66032	0
122	85	5	-1	-4	5	8.80096	3.52681	0.406253	0.0582268
123		5	-1	-4	-5	8.80096	15.6087	0.833437	-0.00159318
124	86	6	-1	-5	3	8.81112	16.0924	0.841805	-0.00909031
125		6	-1	-5	-3	8.81112	12.5804	0.806543	-0.0176241
126	87	6	0	-6	1	8.8162	14.1932	0.81808	-1.05E-09
127		6	0	-6	-1	8.8162	4.57865	0.532832	4.01E-10
128	88	6	-3	-3	4	8.85175	9.41377	0.757459	-0.03587
129	89	7	-3	-4	0	8.86185	5.05922	0.589443	-0.0339885
130	90	3	-1	-2	7	8.90566	13.6203	0.815452	0.00350734
131		3	-1	-2	-7	8.90566	9.32254	0.723219	0.0356358
132	91	7	-3	-4	1	8.93576	13.4745	0.827146	-0.019539
133		7	-3	-4	-1	8.93576	10.2308	0.766717	-0.00905179
134	92	6	-2	-4	4	8.97084	10.2342	0.775044	-0.0157895
135		6	-2	-4	-4	8.97084	7.99688	0.724952	-0.0280241
136	93	4	0	-4	6	9.0174	10.7959	0.78341	-2.90E-09
137		4	0	-4	-6	9.0174	15.213	0.83953	5.56E-10
138	94	6	0	-6	2	9.03723	10.4256	0.772753	2.75E-09
139		6	0	-6	-2	9.03723	7.34609	0.701485	-4.89E-09
140	95	7	-2	-5	0	9.09821	2.27636	0.301837	-0.0220148
141	96	3	0	-3	7	9.14089	7.67184	0.712926	-1.12E-09
142		3	0	-3	-7	9.14089	17.0177	0.860715	4.40E-09
143	97	7	-3	-4	2	9.1539	4.80172	0.597048	-0.0246652
144		7	-3	-4	-2	9.1539	13.9161	0.819226	0.0279956
145	98	7	-2	-5	1	9.17021	3.41618	0.44535	0.0366263
146		7	-2	-5	-1	9.17021	17.1638	0.860835	0.00467805
147	99	5	0	-5	5	9.27075	13.7516	0.838103	1.72E-10
148		5	0	-5	-5	9.27075	3.02413	0.429457	9.81E-09
149	100	1	0	-1	8	9.29013	14.2885	0.842756	-4.65E-09
150		1	0	-1	-8	9.29013	6.79427	0.698727	-5.86E-09
151	101	6	-1	-5	4	9.31898	3.08332	0.46431	-0.00513615
152		6	-1	-5	-4	9.31898	9.00584	0.756303	0.0105097
153	102	5	-2	-3	6	9.36381	3.54474	0.517058	-0.0262577
154		5	-2	-3	-6	9.36381	2.50736	0.355908	0.0306102
155	103	7	-2	-5	2	9.38291	14.0229	0.852513	-0.0140252
156		7	-2	-5	-2	9.38291	7.78045	0.734722	-0.00282402
157	104	6	0	-6	3	9.39406	7.32767	0.725372	1.08E-09
158		6	0	-6	-3	9.39406	13.2267	0.835368	-1.86E-11



159	105	4	-2	-2	7	keV 9.48279	meV 2.08774	0.373145	-0.124963
160	106	6	-3	-3	5	9.49694	8.94336	0.781307	-0.0180603
161	107	7	-3	-4	3	9.50636	8.65494	0.770695	-0.00952812
162		7	-3	-4	-3	9.50636	4.48268	0.566542	0.0646211
163	108	2	-1	-1	8	9.51585	6.26366	0.66134	0.0717716
164	109	7	-1	-6	0	9.5534	11.4321	0.824041	-0.00689129
165	110	5	-1	-4	6	9.5878	12.7696	0.837408	0.0023724
166		5	-1	-4	-6	9.5878	2.5942	0.44785	-0.0470917
167	111	4	-1	-3	7	9.59405	11.1005	0.830417	-0.0247454
168		4	-1	-3	-7	9.59405	6.87335	0.702215	0.0406826
169	112	6	-2	-4	5	9.60804	6.56681	0.716778	-0.00870103
170		6	-2	-4	-5	9.60804	7.1072	0.746165	-0.026618
171	113	7	-1	-6	1	9.622	6.47023	0.710123	0.00811123
172		7	-1	-6	-1	9.622	6.15202	0.708612	-0.0232374
173	114	2	0	-2	8	9.62673	4.49795	0.608237	1.67E-08
174	115	7	-2	-5	3	9.72707	4.27069	0.591564	0.0199658
175		7	-2	-5	-3	9.72707	2.03963	0.345342	-0.0327345
176	116	7	-1	-6	2	9.82492	4.71575	0.625626	0.0342328
177		7	-1	-6	-2	9.82492	11.8761	0.852798	-0.0269842
178	117	6	0	-6	4	9.87198	9.38972	0.804775	1.84E-09
179	118	4	0	-4	7	9.92035	8.87273	0.795577	-3.90E-09
180		4	0	-4	-7	9.92035	2.23827	0.396096	3.90E-08
181	119	6	-1	-5	5	9.93387	7.11545	0.7465	0.0107988
182		6	-1	-5	-5	9.93387	3.4235	0.556996	0.00948394
183	120	3	-1	-2	8	9.95196	8.27714	0.78298	0.0020167
184		3	-1	-2	-8	9.95196	9.11	0.795641	0.0180861
185	121	7	-3	-4	4	9.9789	9.66069	0.820795	-0.00945136
186		7	-3	-4	-4	9.9789	2.34501	0.362447	0.112576
187	122	5	0	-5	-6	10.0208	2.14133	0.384095	-1.08E-08
188	123	8	-4	-4	0	10.0936	6.72816	0.787837	-0.0732174
189	124	7	-1	-6	3	10.1541	5.54281	0.682523	0.062292
190		7	-1	-6	-3	10.1541	5.81262	0.743654	-0.037479
191	125	8	-4	-4	1	10.1585	4.36924	0.674954	-0.0423877
192	126	3	0	-3	8	10.163	13.8585	0.873654	-1.65E-10
193		3	0	-3	-8	10.163	1.73968	0.321571	-3.41E-08
194	127	7	-2	-5	4	10.1894	4.00133	0.632124	-0.0163452
195		7	-2	-5	-4	10.1894	7.26537	0.771759	0.0135358
196	128	8	-3	-5	0	10.1982	8.2856	0.80985	-0.0163044
197		7	0	-7	0	10.1982	7.0604	0.765523	0
198	129	6	-3	-3	6	10.2304	8.1859	0.799496	0.000947975
199	130	5	-2	-3	7	10.2363	1.76294	0.29785	0.068171
200		5	-2	-3	-7	10.2363	6.26139	0.758086	-0.012607
201	131	8	-3	-5	-1	10.2624	2.20165	0.411369	0.0321993
202		7	0	-7	1	10.2624	2.55681	0.481777	1.21E-09

203		7	0	-7	-1	keV 10.2624	meV 11.1385	0.850186	-5.98E-10
204	132	0	0	0	9	10.3221	15.7662	0.892777	1.11E-16
205	133	6	-2	-4	6	10.3336	8.23285	0.787545	0.0352264
206		6	-2	-4	-6	10.3336	6.53645	0.795686	-0.0675514
207	134	8	-4	-4	2	10.3509	8.18272	0.800087	0.00852978
208	135	1	0	-1	9	10.4244	2.90925	0.547105	-9.81E-09
209		1	0	-1	-9	10.4244	4.95041	0.70141	-1.14E-08
210	136	5	-1	-4	7	10.4415	5.95812	0.757856	-0.0136148
211		5	-1	-4	-7	10.4415	4.69863	0.697457	-0.015897
212	137	8	-3	-5	2	10.4529	5.63216	0.731429	0.00362212
213		8	-3	-5	-2	10.4529	4.53944	0.683835	-0.00424069
214		7	0	-7	2	10.4529	7.29304	0.793014	-5.56E-10
215	138	6	0	-6	-5	10.4544	8.66275	0.819547	2.64E-10
216	139	4	-2	-2	8	10.4716	3.52193	0.633118	-0.0414679
217	140	8	-2	-6	0	10.5057	3.96499	0.620022	0.0625727
218	141	7	-3	-4	5	10.5554	2.01615	0.372636	0.10667
219		7	-3	-4	-5	10.5554	7.94649	0.822662	-0.0227736
220	142	8	-2	-6	1	10.5681	6.6568	0.786958	-0.0141537
221		8	-2	-6	-1	10.5681	7.33756	0.798871	-0.00840798
222	143	4	-1	-3	8	10.5724	5.74075	0.765844	-0.0382932
223		4	-1	-3	-8	10.5724	4.98566	0.7213	-0.00707664
224	144	7	-1	-6	4	10.5978	6.89781	0.766203	0.041316
225		7	-1	-6	-4	10.5978	3.2192	0.593302	0.00692787
226	145	2	-1	-1	9	10.626	4.34282	0.657735	0.0519861
227	146	6	-1	-5	6	10.6372	6.18873	0.774091	-0.0100252
228		6	-1	-5	-6	10.6372	8.71335	0.829944	-0.0025449
229	147	8	-4	-4	3	10.6639	6.0464	0.743282	0.0401129
230	148	2	0	-2	9	10.7255	8.72209	0.83397	-7.20E-09
231		2	0	-2	-9	10.7255	6.31222	0.78033	4.02E-09
232	149	8	-2	-6	2	10.7532	3.07607	0.561446	0.0686665
233		8	-2	-6	-2	10.7532	7.79728	0.82079	-0.00850556
234	150	7	-2	-5	5	10.7546	6.45814	0.775509	0.0211447
235		7	-2	-5	-5	10.7546	1.78143	0.411259	-0.0271158
236	151	8	-3	-5	3	10.7629	11.4106	0.871425	-0.00141768
237		8	-3	-5	-3	10.7629	6.75265	0.781255	0.0250133
238	152	5	0	-5	-7	10.8405	11.2604	0.872023	3.51E-11
239	153	4	0	-4	8	10.8694	2.3102	0.51029	-1.80E-08
240		4	0	-4	-8	10.8694	8.76146	0.837862	2.53E-09
241	154	8	-1	-7	0	10.9992	7.69125	0.829615	-0.00874235
242	155	3	-1	-2	9	11.0183	2.61614	0.537827	0.0589079
243	156	6	-3	-3	7	11.0345	1.42334	0.327447	0.0379562
244	157	8	-2	-6	3	11.0548	5.78646	0.774592	0.00229327
245		8	-2	-6	-3	11.0548	4.32356	0.739893	-0.054858
246	158	8	-1	-7	1	11.0588	4.12858	0.722693	-0.0425556

247		8	-1	-7	-1	keV 11.0588	meV 4.58302	0.730437	-0.0101837
248	159	8	-4	-4	4	11.0872	5.81099	0.77443	0.00970259
249	160	6	0	-6	6	11.1249	7.59066	0.827228	-3.11E-10
250		6	0	-6	-6	11.1249	3.23425	0.645546	-2.66E-09
251	161	6	-2	-4	7	11.1303	6.20625	0.785725	0.0154648
252		6	-2	-4	-7	11.1303	2.91225	0.622524	-0.0223802
253	162	7	-1	-6	5	11.1423	2.93041	0.61921	-0.0115054
254		7	-1	-6	-5	11.1423	5.36202	0.735765	0.06226
255	163	5	-2	-3	8	11.1585	6.61948	0.819806	-0.0217211
256	164	8	-3	-5	4	11.1825	4.05554	0.700469	0.00705186
257		8	-3	-5	-4	11.1825	1.24931	0.33883	-0.0814934
258		7	0	-7	4	11.1825	1.78431	0.442996	8.66E-09
259		7	0	-7	-4	11.1825	8.95692	0.854956	2.13E-09
260	165	3	0	-3	9	11.2093	3.60993	0.675107	1.14E-08
261		3	0	-3	-9	11.2093	1.65591	0.418509	1.95E-08
262	166	7	-3	-4	6	11.2199	2.15699	0.477521	0.08585
263		7	-3	-4	-6	11.2199	5.28329	0.773789	-0.016018
264	167	8	-1	-7	-2	11.2358	2.46325	0.565776	0.00648351
265	168	5	-1	-4	8	11.3471	3.22939	0.661048	-0.0102564
266		5	-1	-4	-8	11.3471	6.23241	0.796985	0.0178038
267	169	9	-4	-5	0	11.3786	1.57299	0.414786	0.0064525
268	170	7	-2	-5	6	11.4075	1.20967	0.333735	-0.0503486
269		7	-2	-5	-6	11.4075	2.58148	0.582698	0.0205017
270	171	6	-1	-5	7	11.4127	5.62344	0.79134	-0.00448602
271		6	-1	-5	-7	11.4127	1.45704	0.415034	-0.0461892
272	172	9	-4	-5	1	11.4363	4.22309	0.726832	0.00741958
273		9	-4	-5	-1	11.4363	6.91618	0.833146	-0.0125759
274	173	8	-2	-6	4	11.4637	6.18091	0.798956	0.0211489
275		8	-2	-6	-4	11.4637	1.14676	0.341139	-0.0819581
276	174	4	-2	-2	9	11.4898	6.56442	0.832021	-0.0220007
277	175	8	-1	-7	3	11.5248	5.56863	0.776983	0.0350125
278		8	-1	-7	-3	11.5248	5.72768	0.809247	-0.0194819
279	176	1	0	-1	10	11.5611	6.09197	0.809825	-3.06E-10
280		1	0	-1	-10	11.5611	6.63869	0.825066	9.11E-09
281	177	9	-3	-6	0	11.5636	3.95225	0.694667	0.056002
282	178	4	-1	-3	9	11.5818	5.89366	0.807827	-0.00494645
283		4	-1	-3	-9	11.5818	6.19949	0.819438	-0.0111031
284	179	9	-4	-5	2	11.6075	6.21303	0.80899	0.0158317
285	180	8	-4	-4	5	11.6088	4.26218	0.741956	0.00427113
286	181	9	-3	-6	1	11.6204	3.87026	0.697091	0.0547451
287		9	-3	-6	-1	11.6204	1.84666	0.501298	0.0152429
288	182	8	0	-8	0	11.655	3.58348	0.704369	0
289	183	8	-3	-5	5	11.6999	1.04348	0.316701	-0.0775638
290		8	-3	-5	-5	11.6999	2.9378	0.650563	0.00943191

291		7	0	-7	5	keV 11.6999	meV 8.22072	0.861194	-1.64E-09
292		7	0	-7	-5	11.6999	1.94814	0.524771	-1.19E-08
293	184	8	0	-8	1	11.7113	6.53993	0.829433	6.49E-10
294	185	5	0	-5	8	11.7152	4.02819	0.743708	-1.09E-09
295	186	2	-1	-1	10	11.7433	2.72336	0.627796	0.0300441
296	187	7	-1	-6	6	11.7737	4.34297	0.776456	-0.0389363
297		7	-1	-6	-6	11.7737	3.9679	0.711825	0.0516169
298	188	9	-3	-6	2	11.7889	4.96672	0.786289	-0.00523728
299		9	-3	-6	-2	11.7889	5.34687	0.796848	0.00298618
300	189	2	0	-2	10	11.8333	1.18681	0.347392	6.74E-08
301		2	0	-2	-10	11.8333	1.23106	0.363469	6.23E-11
302	190	4	0	-4	9	11.8535	5.1851	0.796743	9.30E-09
303		4	0	-4	-9	11.8535	4.36468	0.76443	-1.13E-08
304	191	6	0	-6	7	11.8686	3.2498	0.698636	9.23E-09
305		6	0	-6	-7	11.8686	4.78358	0.779069	-9.61E-09
306	192	8	0	-8	2	11.8786	1.50023	0.448274	-5.05E-09
307		8	0	-8	-2	11.8786	3.72489	0.733784	4.51E-10
308	193	9	-4	-5	3	11.8874	2.33123	0.61153	-0.0204825
309		9	-4	-5	-3	11.8874	2.65719	0.633149	0.0137575
310	194	6	-3	-3	8	11.895	3.624	0.70165	0.0408047
311	195	8	-1	-7	4	11.9176	4.28399	0.745218	0.0299179
312		8	-1	-7	-4	11.9176	3.37146	0.692596	0.0256959
313	196	9	-2	-7	0	11.9251	1.10648	0.361121	-0.0601676
314	197	7	-3	-4	7	11.9577	5.9824	0.812578	0.0248786
315		7	-3	-4	-7	11.9577	3.14412	0.701337	-0.0219448
316	198	8	-2	-6	5	11.9689	1.79162	0.55724	-0.0670943
317		8	-2	-6	-5	11.9689	5.0782	0.786499	0.0225602
318	199	9	-2	-7	1	11.9801	3.43179	0.709475	0.00784285
319		9	-2	-7	-1	11.9801	6.04713	0.81151	0.0324847
320	200	6	-2	-4	8	11.9839	2.85888	0.643833	0.0487184
321		6	-2	-4	-8	11.9839	2.61946	0.640041	0.0149291
322	201	9	-3	-6	3	12.0647	3.63046	0.742431	-0.019788
323		9	-3	-6	-3	12.0647	2.93743	0.710957	-0.0599051
324	202	3	-1	-2	10	12.0994	4.62995	0.781408	0.0119298
325		3	-1	-2	-10	12.0994	3.60406	0.743989	-0.0232143
326	203	5	-2	-3	9	12.1191	3.42905	0.717679	0.00653101
327		5	-2	-3	-9	12.1191	3.61249	0.732421	0.00108893
328	204	7	-2	-5	7	12.1339	2.62856	0.652304	0.00198252
329		7	-2	-5	-7	12.1339	6.84134	0.856942	-0.011257
330	205	9	-2	-7	2	12.1437	5.18653	0.82296	-0.0265359
331		9	-2	-7	-2	12.1437	2.26094	0.604237	0.0151467
332	206	8	0	-8	3	12.1523	2.4178	0.632862	5.09E-10
333		8	0	-8	-3	12.1523	1.1365	0.368994	1.00E-09
334	207	8	-4	-4	6	12.2161	3.28612	0.7094	0.0188991

335	208	6	-1	-5	-8	keV 12.2467	meV 5.63669	0.824291	0.00219276
336	209	9	-4	-5	4	12.2686	4.59611	0.793984	-0.00614759
337		9	-4	-5	-4	12.2686	4.04944	0.768957	0.00208807
338	210	3	0	-3	-10	12.2735	5.99139	0.837337	-5.41E-09
339	211	5	-1	-4	-9	12.293	2.74842	0.673194	0.0125605
340	212	8	-3	-5	6	12.3027	3.59006	0.733699	0.02894
341		8	-3	-5	-6	12.3027	7.30331	0.867413	-0.00517809
342	213	8	-1	-7	5	12.4043	3.64322	0.74186	0.0177087
343		8	-1	-7	-5	12.4043	3.79943	0.749101	0.022225
344	214	9	-2	-7	3	12.4115	1.17125	0.421885	-0.035754
345		9	-2	-7	-3	12.4115	3.77253	0.750619	0.0150851
346	215	9	-3	-6	4	12.4404	4.98456	0.829112	-0.0308077
347		9	-3	-6	-4	12.4404	3.85842	0.764863	0.00185763
348	216	9	-1	-8	0	12.4476	4.66047	0.80895	-0.0131846
349	217	7	-1	-6	7	12.4788	5.20645	0.838756	-0.0332786
350		7	-1	-6	-7	12.4788	2.19576	0.616533	0.0231092
351	218	9	-1	-8	1	12.5003	3.87619	0.794243	-0.0501331
352		9	-1	-8	-1	12.5003	1.77929	0.547266	0.0430777
353	219	8	0	-8	4	12.5254	6.09237	0.848086	-2.08E-09
354		8	0	-8	-4	12.5254	3.62188	0.755158	-5.65E-09
355	220	4	-2	-2	10	12.5303	3.20346	0.729736	-0.00143489
356	221	8	-2	-6	6	12.5588	2.27987	0.67609	-0.061469
357		8	-2	-6	-6	12.5588	3.67767	0.753225	0.0161762
358	222	4	-1	-3	10	12.6147	2.31127	0.630982	0.0503591
359		4	-1	-3	-10	12.6147	3.36187	0.769185	-0.0485222
360	223	10	-5	-5	0	12.617	7.7268	0.880127	0.000814207
361	224	9	-1	-8	2	12.6572	4.14564	0.790785	-0.0021945
362		9	-1	-8	-2	12.6572	2.61854	0.655226	0.0673312
363	225	10	-5	-5	1	12.669	1.36495	0.484605	-0.00385172
364	226	6	0	-6	8	12.6726	2.31698	0.655743	9.26E-09
365		6	0	-6	-8	12.6726	4.00149	0.784954	7.42E-09
366	227	1	0	-1	11	12.6997	3.18747	0.741064	1.98E-08
367		1	0	-1	-11	12.6997	1.30897	0.48088	-3.19E-09
368	228	10	-4	-6	0	12.7008	2.12917	0.637926	-0.00775183
369	229	9	-4	-5	5	12.7419	3.61544	0.773874	-0.00813314
370		9	-4	-5	-5	12.7419	4.70554	0.816887	-0.00401265
371	230	10	-4	-6	1	12.7525	5.17666	0.819529	0.0243637
372		10	-4	-6	-1	12.7525	3.30045	0.755518	-0.0134518
373	231	7	-3	-4	8	12.756	3.63523	0.773512	-0.0118749
374		7	-3	-4	-8	12.756	4.40134	0.809168	-0.00540589
375	232	9	-2	-7	4	12.7771	0.848513	0.354733	-0.0982054
376		9	-2	-7	-4	12.7771	4.68276	0.827136	-0.0187744
377	233	6	-3	-3	9	12.8005	4.3218	0.806056	-0.00289497
378	234	4	0	-4	10	12.8646	3.40662	0.760491	1.76E-10

379		4	0	-4	-10	keV 12.8646	meV 1.84005	0.601509	-5.29E-09
380	235	2	-1	-1	11	12.8658	4.36571	0.811457	-0.00684005
381	236	6	-2	-4	9	12.8831	4.15846	0.799913	0.00149163
382		6	-2	-4	-9	12.8831	4.78711	0.811943	0.0241768
383	237	8	-4	-4	7	12.897	3.48141	0.765302	0.00399585
384	238	10	-4	-6	2	12.9063	1.04544	0.402451	0.0240237
385		10	-4	-6	-2	12.9063	3.47521	0.790461	-0.0437132
386	239	9	-3	-6	5	12.9074	2.82281	0.719326	0.00534596
387		9	-3	-6	-5	12.9074	3.9768	0.808767	-0.0301065
388	240	9	-1	-8	3	12.9144	2.73304	0.718868	-0.00526751
389		9	-1	-8	-3	12.9144	2.72578	0.696685	0.0376054
390	241	7	-2	-5	8	12.9214	5.97524	0.858223	-9.68E-05
391		7	-2	-5	-8	12.9214	0.852842	0.293973	0.0501134
392	242	2	0	-2	11	12.948	1.08836	0.422798	1.75E-09
393		2	0	-2	-11	12.948	3.0611	0.740245	1.05E-08
394	243	10	-3	-7	0	12.949	4.18045	0.794808	0.0222344
395	244	8	-1	-7	6	12.9744	4.02476	0.812421	-0.0259721
396		8	-1	-7	-6	12.9744	3.8281	0.773855	0.0332403
397	245	8	-3	-5	7	12.9791	1.74264	0.598091	-0.00939936
398		8	-3	-5	-7	12.9791	2.86532	0.723545	0.006967
399		7	0	-7	-7	12.9791	3.40517	0.770348	-1.89E-09
400	246	8	0	-8	5	12.9894	2.88503	0.729209	7.76E-09
401		8	0	-8	-5	12.9894	5.77214	0.855448	1.67E-09
402	247	10	-3	-7	1	12.9997	1.20245	0.482577	-0.033074
403	248	10	-5	-5	3	13.0777	3.21678	0.764732	-0.0019031
404	249	5	-2	-3	10	13.1097	0.958488	0.396974	-0.018789
405		5	-2	-3	-10	13.1097	5.11685	0.84624	-0.00659227
406	250	9	0	-9	0	13.1119	0.800522	0.319532	5.55E-17
407	251	6	-1	-5	9	13.1279	2.90986	0.727374	0.029814
408		6	-1	-5	-9	13.1279	2.38509	0.67729	0.038337
409	252	10	-3	-7	2	13.1506	2.37085	0.681867	0.0173421
410		10	-3	-7	-2	13.1506	1.39429	0.538179	-0.0129293
411	253	10	-4	-6	3	13.1586	1.92671	0.645657	-0.0195988
412		10	-4	-6	-3	13.1586	1.26623	0.473449	0.0539457
413	254	9	0	-9	1	13.162	2.01281	0.647784	1.07E-09
414		9	0	-9	-1	13.162	3.62454	0.788749	8.21E-10
415	255	3	-1	-2	11	13.1916	1.52302	0.539354	0.0555725
416		3	-1	-2	-11	13.1916	4.01978	0.811931	-0.00820846
417	256	8	-2	-6	7	13.2221	3.68948	0.801699	-0.0158179
418		8	-2	-6	-7	13.2221	2.07329	0.642005	0.0377923
419	257	9	-2	-7	5	13.2322	4.15999	0.818092	-0.00515287
420		9	-2	-7	-5	13.2322	0.815994	0.377193	-0.08577
421	258	7	-1	-6	8	13.2458	2.05419	0.667265	-0.014933
422		7	-1	-6	-8	13.2458	2.61875	0.73714	-0.02603

423	259	9	-1	-8	4	keV 13.2661	meV 2.65531	0.710803	0.0314516
424		9	-1	-8	-4	13.2661	2.72231	0.740167	-0.015194
425	260	5	-1	-4	10	13.2706	4.26552	0.813221	0.0142145
426		5	-1	-4	-10	13.2706	1.33323	0.522418	0.00972913
427	261	9	-4	-5	6	13.2976	1.65673	0.590098	0.0193288
428		9	-4	-5	-6	13.2976	1.38831	0.556088	-0.0267612
429	262	9	0	-9	2	13.311	3.524	0.789737	1.04E-09
430		9	0	-9	-2	13.311	0.805556	0.33628	7.73E-10
431	263	3	0	-3	11	13.3515	3.57252	0.794339	-8.63E-09
432		3	0	-3	-11	13.3515	2.56945	0.721803	5.64E-09
433	264	10	-2	-8	0	13.3525	1.82425	0.627378	0.00897617
434	265	10	-3	-7	3	13.3984	3.3977	0.807131	-0.0397729
435		10	-3	-7	-3	13.3984	5.18093	0.851622	0.00398262
436	266	10	-2	-8	1	13.4017	4.67487	0.843751	-0.00881841
437	267	9	-3	-6	6	13.4563	1.65122	0.634514	-0.0454037
438		9	-3	-6	-6	13.4563	2.44362	0.715718	0.00211977
439	268	10	-4	-6	4	13.5039	2.40812	0.7278	-0.0173693
440		10	-4	-6	-4	13.5039	3.20537	0.773444	0.00866802
441	269	6	0	-6	9	13.5261	1.33363	0.553509	-3.21E-09
442		6	0	-6	-9	13.5261	2.25247	0.702546	2.82E-09
443	270	8	0	-8	6	13.5349	0.893439	0.401869	-2.22E-09
444		8	0	-8	-6	13.5349	1.96002	0.664523	-7.84E-10
445	271	10	-2	-8	2	13.5481	2.11398	0.686732	-0.00414793
446		10	-2	-8	-2	13.5481	4.24382	0.817776	0.0240346
447	272	9	0	-9	3	13.5558	3.84302	0.812066	-1.30E-09
448		9	0	-9	-3	13.5558	0.956058	0.431646	-9.10E-09
449	273	5	0	-5	-10	13.5868	1.88792	0.668787	1.27E-09
450	274	7	-3	-4	9	13.6043	1.7407	0.65123	-0.030637
451		7	-3	-4	-9	13.6043	0.880669	0.404299	-0.00286714
452	275	8	-1	-7	7	13.6175	1.17469	0.532354	-0.0388476
453		8	-1	-7	-7	13.6175	0.656007	0.328945	-0.103253
454	276	8	-4	-4	8	13.6405	1.75177	0.657884	-0.0292634
455	277	4	-1	-3	11	13.6658	2.19005	0.672328	0.0578786
456		4	-1	-3	-11	13.6658	3.55996	0.811401	-0.0145103
457	278	9	-1	-8	5	13.705	1.95982	0.684012	-0.0149081
458		9	-1	-8	-5	13.705	2.39016	0.722733	0.00432805
459	279	8	-3	-5	8	13.7181	1.36125	0.556477	0.0203487
460		7	0	-7	8	13.7181	3.65967	0.812648	6.03E-09
461		7	0	-7	-8	13.7181	0.69476	0.308778	3.68E-09
462	280	10	-3	-7	4	13.7377	1.1146	0.475884	0.0461561
463		10	-3	-7	-4	13.7377	1.50421	0.605785	-0.0123984
464	281	6	-3	-3	10	13.7421	2.79835	0.752281	0.0164403
465	282	7	-2	-5	9	13.7595	0.75202	0.34478	0.00439089
466	283	0	0	0	12	13.7628	1.91054	0.681352	6.66E-16

467	284	9	-2	-7	6	keV 13.7681	meV 2.49262	0.728703	0.0146857
468		9	-2	-7	-6	13.7681	0.667845	0.338633	-0.0797263
469	285	10	-2	-8	-3	13.7887	1.36386	0.589999	-0.0355186
470	286	6	-2	-4	10	13.8191	1.25622	0.567406	-0.0272008
471		6	-2	-4	-10	13.8191	1.93208	0.658566	0.0382178
472	287	1	0	-1	-12	13.8397	1.40688	0.586645	-8.90E-09
473	288	9	0	-9	4	13.8913	0.811794	0.392471	-1.31E-08
474		9	0	-9	-4	13.8913	3.66591	0.818372	-1.28E-09
475	289	4	0	-4	11	13.8968	0.930378	0.446817	-1.10E-08
476		4	0	-4	-11	13.8968	1.15985	0.530503	1.58E-09
477	290	11	-5	-6	0	13.8977	2.02544	0.692195	0.00293442
478		10	-1	-9	0	13.8977	2.69798	0.7835	-0.0416891
479	291	9	-4	-5	-7	13.9257	3.41872	0.80285	0.0101299
480	292	10	-4	-6	5	13.9354	3.20712	0.793325	0.00446382
481		10	-4	-6	-5	13.9354	2.41247	0.735827	0.00941724
482	293	11	-5	-6	1	13.945	2.73036	0.762565	0.00652883
483		11	-5	-6	-1	13.945	3.30813	0.809185	-0.0141513
484		10	-1	-9	1	13.945	1.4673	0.59935	0.0150196
485		10	-1	-9	-1	13.945	2.90405	0.778115	-0.00214786
486	294	8	-2	-6	8	13.9483	2.75222	0.76653	-0.000824436
487		8	-2	-6	-8	13.9483	2.61643	0.768707	-0.0205817
488	295	2	-1	-1	12	13.9922	1.87011	0.697561	-0.0371526
489	296	6	-1	-5	10	14.0476	2.67442	0.762841	0.00566248
490		6	-1	-5	-10	14.0476	0.944712	0.467034	-0.00329131
491	297	11	-4	-7	0	14.0496	1.36012	0.603266	-0.0245929
492	298	7	-1	-6	9	14.0646	2.90626	0.7806	0.00459205
493		7	-1	-6	-9	14.0646	3.06019	0.80019	-0.0154501
494	299	2	0	-2	12	14.0678	4.29632	0.848077	1.57E-09
495		2	0	-2	-12	14.0678	3.33889	0.809753	-8.92E-09
496	300	9	-3	-6	7	14.0773	2.57279	0.749788	0.0203327
497		9	-3	-6	-7	14.0773	2.23669	0.73129	-0.00588026
498	301	11	-5	-6	2	14.0858	2.17898	0.711954	0.024399
499		11	-5	-6	-2	14.0858	1.45748	0.629599	-0.0214535
500		10	-1	-9	2	14.0858	1.882	0.677298	0.0184556
501		10	-1	-9	-2	14.0858	1.08744	0.509741	0.0186193
502	302	11	-4	-7	1	14.0964	1.30756	0.591866	-0.0134165
503		11	-4	-7	-1	14.0964	2.0609	0.74349	-0.0629382
504	303	10	-2	-8	4	14.1186	2.10109	0.735364	-0.0300733
505		10	-2	-8	-4	14.1186	1.27225	0.562059	0.0229639
506	304	5	-2	-3	11	14.124	2.64846	0.764032	0.0116559
507		5	-2	-3	-11	14.124	0.914148	0.450308	0.0136397
508	305	8	0	-8	7	14.1525	1.89431	0.697292	3.85E-09
509	306	10	-3	-7	5	14.162	1.01037	0.513073	-0.0318183
510		10	-3	-7	-5	14.162	0.915944	0.437255	0.0467157



511	307	9	-1	-8	6	keV 14.2231	meV 2.10471	0.709754	0.0255283
512		9	-1	-8	-6	14.2231	2.17752	0.737897	-0.0151832
513	308	11	-4	-7	2	14.2357	2.71641	0.78154	-0.00781308
514		11	-4	-7	-2	14.2357	2.52465	0.766484	-0.00905339
515	309	5	-1	-4	11	14.2735	1.21302	0.572813	-0.00759365
516		5	-1	-4	-11	14.2735	2.14591	0.744432	-0.0272674
517	310	3	-1	-2	12	14.2924	2.38639	0.751791	-0.000233898
518		3	-1	-2	-12	14.2924	1.73771	0.68776	-0.0230661
519	311	9	0	-9	5	14.3111	3.26372	0.813958	5.12E-10
520		9	0	-9	-5	14.3111	0.924657	0.477226	8.68E-09
521	312	11	-5	-6	-3	14.3173	1.66358	0.661533	0.00838042
522		10	-1	-9	3	14.3173	2.69783	0.767131	0.0259635
523		10	-1	-9	-3	14.3173	3.25295	0.807864	0.0109767
524	313	8	-1	-7	8	14.3236	1.37534	0.62464	-0.02549
525		8	-1	-7	-8	14.3236	1.47134	0.659189	-0.0528233
526	314	11	-3	-8	0	14.3486	0.980616	0.549809	-0.0925207
527	315	10	-5	-5	6	14.3715	2.88547	0.796095	-0.000431617
528	316	9	-2	-7	7	14.3757	1.60209	0.651181	0.0150417
529		9	-2	-7	-7	14.3757	2.76643	0.793176	-0.0108884
530	317	11	-3	-8	1	14.3944	2.42234	0.750207	0.0194028
531		11	-3	-8	-1	14.3944	2.21909	0.735513	0.0153537
532	318	6	0	-6	10	14.4204	2.96815	0.800928	-8.07E-09
533	319	8	-4	-4	9	14.4369	1.83897	0.730389	-0.0621662
534	320	3	0	-3	12	14.4401	0.894797	0.474254	1.60E-08
535	321	10	-4	-6	6	14.4452	0.926051	0.46334	0.0510225
536		10	-4	-6	-6	14.4452	1.51503	0.658213	-0.0216374
537	322	11	-4	-7	3	14.4648	1.11223	0.537316	0.0342283
538		11	-4	-7	-3	14.4648	1.48184	0.642802	-0.0003284
539	323	7	-3	-4	10	14.4938	2.66231	0.797338	-0.0249563
540		7	-3	-4	-10	14.4938	1.61969	0.668899	-0.00103342
541	324	8	-3	-5	9	14.5103	2.90101	0.808227	-0.0139314
542		8	-3	-5	-9	14.5103	2.04501	0.736718	-0.00866202
543		7	0	-7	9	14.5103	1.85906	0.703829	-1.10E-08
544		7	0	-7	-9	14.5103	1.84337	0.701733	9.43E-09
545	325	11	-3	-8	2	14.5308	2.5676	0.787329	-0.0173291
546		11	-3	-8	-2	14.5308	1.50462	0.68002	-0.0565251
547	326	10	-2	-8	5	14.5318	0.867753	0.45564	0.0308738
548		10	-2	-8	-5	14.5318	2.01338	0.751685	-0.0435767
549	327	5	0	-5	11	14.5679	4.65091	0.87177	1.66E-10
550	328	10	0	-10	1	14.6139	1.7935	0.708443	-2.97E-10
551	329	9	-4	-5	8	14.617	2.94144	0.810299	-0.00650898
552		9	-4	-5	-8	14.617	1.09638	0.552463	0.0179975
553	330	11	-5	-6	4	14.6353	2.3118	0.761481	9.89E-05
554		11	-5	-6	-4	14.6353	1.59329	0.669946	0.0114826

555		10	-1	-9	4	keV 14.6353	meV 1.08993	0.57631	-0.035063
556	331	7	-2	-5	10	14.6395	0.666039	0.362547	0.0225002
557		7	-2	-5	-10	14.6395	3.20334	0.818054	0.00870863
558	332	4	-2	-2	12	14.6589	2.5927	0.776054	0.0204312
559	333	10	-3	-7	6	14.6639	3.73743	0.840899	0.0101507
560		10	-3	-7	-6	14.6639	2.18038	0.77273	-0.0392158
561	334	6	-3	-3	11	14.7128	0.757581	0.473777	-0.0751328
562	335	8	-2	-6	9	14.728	1.48224	0.634892	0.0475211
563		8	-2	-6	-9	14.728	0.959132	0.505772	0.0377055
564	336	4	-1	-3	12	14.7311	1.10471	0.554476	0.0391153
565		4	-1	-3	-12	14.7311	1.1726	0.586184	0.0132717
566	337	10	0	-10	-2	14.7483	3.94474	0.855778	-1.72E-10
567	338	11	-3	-8	3	14.7554	1.70664	0.681716	0.0302353
568		11	-3	-8	-3	14.7554	2.13255	0.745428	0.00636021
569	339	9	-3	-6	8	14.7615	0.937821	0.519588	0.00244191
570		9	-3	-6	-8	14.7615	1.7245	0.674911	0.0542187
571	340	11	-4	-7	4	14.7797	1.89041	0.714758	0.0175844
572		11	-4	-7	-4	14.7797	2.98053	0.797604	0.0333893
573	341	6	-2	-4	11	14.7848	1.32238	0.65035	-0.0422627
574		6	-2	-4	-11	14.7848	2.4576	0.776456	0.00586835
575	342	11	-2	-9	0	14.7857	2.21143	0.758783	-0.00157393
576	343	9	0	-9	-6	14.808	2.63592	0.792763	2.91E-09
577	344	9	-1	-8	7	14.812	1.26429	0.599971	0.0380572
578		9	-1	-8	-7	14.812	2.07107	0.74402	0.00275492
579	345	11	-2	-9	1	14.8301	1.29265	0.611539	0.027529
580		11	-2	-9	-1	14.8301	1.89232	0.734118	-0.0126327
581	346	8	0	-8	-8	14.8332	2.33972	0.773769	-6.94E-09
582	347	7	-1	-6	10	14.9267	1.38091	0.631146	0.043738
583		7	-1	-6	-10	14.9267	1.30322	0.644371	-0.0226352
584	348	4	0	-4	12	14.9457	2.70859	0.804242	-6.51E-09
585		4	0	-4	-12	14.9457	2.36304	0.779479	9.29E-09
586	349	10	-5	-5	7	14.9546	0.654498	0.393262	-0.000966791
587	350	11	-2	-9	2	14.9626	2.80823	0.796682	0.0278337
588		11	-2	-9	-2	14.9626	1.55985	0.6987	-0.0286805
589	351	10	0	-10	-3	14.9696	1.15052	0.596258	3.66E-09
590	352	1	0	-1	13	14.9807	1.79094	0.720375	-4.76E-09
591		1	0	-1	-13	14.9807	1.54913	0.687471	-1.65E-08
592	353	6	-1	-5	11	14.9986	1.13206	0.594265	0.00102298
593		6	-1	-5	-11	14.9986	1.22521	0.628197	-0.0125473
594	354	10	-2	-8	6	15.0214	1.17896	0.620723	-0.0256599
595		10	-2	-8	-6	15.0214	0.570753	0.312464	0.0620405
596	355	10	-4	-6	7	15.0254	2.15738	0.775284	-0.0218696
597		10	-4	-6	-7	15.0254	0.590324	0.370764	-0.00783289
598	356	11	-5	-6	5	15.0344	1.62186	0.702105	-0.00318358

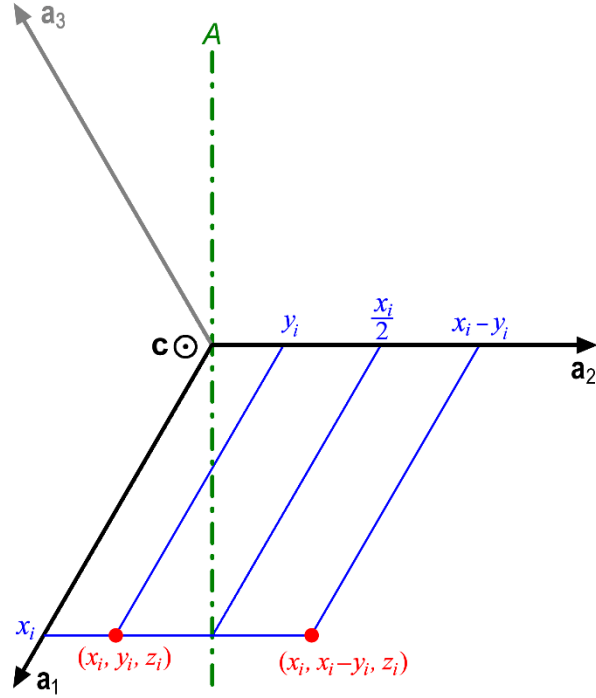
599		11	-5	-6	-5	keV 15.0344	meV 2.29121	0.774558	0.00273683
600	357	10	-1	-9	5	15.0344	0.540273	0.364286	-0.0732295
601		10	-1	-9	-5	15.0344	1.03027	0.582406	-0.0307354
602	358	9	-2	-7	8	15.0463	2.52418	0.783042	0.0255804
603		9	-2	-7	-8	15.0463	1.62341	0.693258	0.0101059
604	359	11	-3	-8	4	15.0641	0.933323	0.533476	0.0110138
605		11	-3	-8	-4	15.0641	2.04169	0.752505	0.00397993
606	360	8	-1	-7	9	15.084	2.39627	0.785915	0.00278441
607		8	-1	-7	-9	15.084	2.47899	0.801335	-0.0156776
608	361	2	-1	-1	13	15.1217	2.36408	0.795181	-0.0199942
609	362	12	-6	-6	0	15.1403	0.646286	0.398509	0.0162435
610	363	11	-4	-7	5	15.1749	2.46568	0.778919	0.0327279
611		11	-4	-7	-5	15.1749	1.48792	0.673087	0.0229173
612	364	11	-2	-9	3	15.1808	1.09607	0.596287	0.00445417
613		11	-2	-9	-3	15.1808	0.969416	0.559354	0.000657959
614	365	12	-6	-6	1	15.1837	1.32675	0.635848	0.0398674
615	366	2	0	-2	13	15.1917	1.37574	0.662137	-7.68E-09
616	367	12	-5	-7	0	15.2103	2.25627	0.786645	-0.00966648
617	368	10	-3	-7	7	15.2358	0.861255	0.529879	-0.0218593
618		10	-3	-7	-7	15.2358	1.0736	0.58142	0.0213972
619	369	12	-5	-7	1	15.2535	0.739814	0.45611	0.015252
620		12	-5	-7	-1	15.2535	0.792409	0.484415	0.0105091
621	370	10	0	-10	4	15.274	2.91303	0.827568	1.40E-12
622		10	0	-10	-4	15.274	0.651615	0.416815	-4.34E-09
623	371	8	-4	-4	10	15.278	1.06442	0.611075	-0.0287343
624	372	5	-1	-4	12	15.2966	1.42566	0.683379	-0.00798538
625		5	-1	-4	-12	15.2966	2.28491	0.785302	-0.00093901
626	373	12	-6	-6	2	15.3131	2.02713	0.756435	0.0124511
627	374	8	-3	-5	10	15.3473	0.484595	0.303434	0.00081659
628		7	0	-7	10	15.3473	0.727717	0.4652	1.48E-08
629		7	0	-7	-10	15.3473	2.87517	0.827706	-3.00E-09
630	375	6	0	-6	11	15.3483	1.37608	0.671199	1.02E-08
631		6	0	-6	-11	15.3483	1.32585	0.665215	-2.11E-08
632	376	11	-1	-10	0	15.3492	1.19647	0.646753	-0.0226617
633	377	9	-4	-5	9	15.3629	0.560281	0.371199	-0.0112035
634		9	-4	-5	-9	15.3629	0.628751	0.403901	0.0164457
635	378	9	0	-9	7	15.3745	0.614825	0.403822	6.06E-09
636		9	0	-9	-7	15.3745	1.95258	0.758856	-1.39E-09
637	379	12	-5	-7	-2	15.3823	1.26852	0.654115	-0.00884795
638	380	11	-1	-10	1	15.392	0.753242	0.482737	0.00248782
639		11	-1	-10	-1	15.392	2.25947	0.799924	-0.0257848
640	381	3	-1	-2	13	15.3999	2.21019	0.7897	-0.0116773
641	382	7	-3	-4	11	15.4173	0.479385	0.304418	0.000965606
642		7	-3	-4	-11	15.4173	2.27418	0.779876	0.020187

643	383	12	-4	-8	0	keV 15.4182	meV 0.463117	0.267619	0.0429716
644	384	11	-3	-8	5	15.4521	1.78557	0.736286	0.0117833
645		11	-3	-8	-5	15.4521	1.08106	0.594289	0.0314915
646	385	12	-4	-8	1	15.4608	1.9769	0.778642	-0.0280343
647		12	-4	-8	-1	15.4608	1.11099	0.613846	0.00822063
648	386	9	-1	-8	8	15.4637	1.01823	0.580061	0.0264623
649		9	-1	-8	-8	15.4637	1.50359	0.722813	-0.0437683
650	387	11	-2	-9	4	15.4811	0.790554	0.502871	0.0111983
651		11	-2	-9	-4	15.4811	1.72606	0.753968	-0.0360168
652	388	9	-3	-6	9	15.5004	1.41063	0.66557	0.0414545
653		9	-3	-6	-9	15.5004	1.13993	0.605598	0.0447796
654	389	11	-5	-6	6	15.5081	1.52922	0.702524	0.00744474
655		10	-1	-9	6	15.5081	2.29586	0.794293	0.000753077
656		10	-1	-9	-6	15.5081	1.79484	0.738636	0.0151711
657	390	11	-1	-10	2	15.5196	1.31699	0.647416	0.0489934
658		11	-1	-10	-2	15.5196	1.46568	0.690925	0.010978
659	391	12	-6	-6	3	15.5264	1.0696	0.611721	-0.00400842
660	392	3	0	-3	13	15.5371	1.08442	0.614038	-9.12E-09
661		3	0	-3	-13	15.5371	1.47906	0.704879	-1.39E-09
662	393	8	-2	-6	10	15.5534	1.68362	0.734507	-0.00111052
663		8	-2	-6	-10	15.5534	1.60966	0.727932	-0.013935
664	394	7	-2	-5	11	15.5543	2.14642	0.790369	-0.0109734
665		7	-2	-5	-11	15.5543	1.4107	0.689914	-0.00450927
666	395	8	0	-8	9	15.5687	1.29794	0.667434	1.44E-10
667		8	0	-8	-9	15.5687	1.04669	0.605805	7.15E-10
668	396	10	-2	-8	7	15.5802	2.72502	0.817328	0.0176946
669		10	-2	-8	-7	15.5802	1.08809	0.622269	-0.00945745
670	397	12	-4	-8	2	15.5879	1.36989	0.693525	-0.0210728
671		12	-4	-8	-2	15.5879	2.02704	0.775131	-0.00128394
672	398	12	-5	-7	3	15.5946	2.75904	0.829114	-0.00066865
673		12	-5	-7	-3	15.5946	2.28124	0.792207	0.0104424
674	399	10	-5	-5	8	15.6004	0.706395	0.473741	-0.00276183
675	400	11	-4	-7	6	15.6444	1.11387	0.632915	-0.00835967
676		11	-4	-7	-6	15.6444	0.762093	0.492496	0.0270937
677	401	10	0	-10	5	15.6568	0.65894	0.450345	5.24E-09
678		10	0	-10	-5	15.6568	2.24042	0.79637	3.08E-10
679	402	10	-4	-6	8	15.6682	1.16424	0.653191	-0.0175458
680		10	-4	-6	-8	15.6682	2.28934	0.791772	0.0153084
681	403	6	-3	-3	12	15.7074	1.66211	0.736083	0.00313356
682	404	11	-1	-10	3	15.7301	1.96498	0.769683	0.00543907
683		11	-1	-10	-3	15.7301	1.27327	0.667952	0.00951543
684	405	4	-2	-2	13	15.7407	0.993643	0.588528	0.0226605
685	406	12	-3	-9	0	15.7586	2.0445	0.769816	0.0255703
686	407	9	-2	-7	-9	15.7719	0.638806	0.450903	-0.00340132

687	408	6	-2	-4	12	keV 15.7748	meV 1.22543	0.692924	-0.0546999
688		6	-2	-4	-12	15.7748	1.29493	0.680467	-0.00031808
689	409	12	-4	-8	3	15.7974	1.44783	0.714087	-0.0152844
690		12	-4	-8	-3	15.7974	0.581438	0.400827	0.0277196
691	410	12	-3	-9	1	15.8002	0.78944	0.535395	-0.0152915
692		12	-3	-9	-1	15.8002	0.789899	0.521638	0.0145712
693	411	4	-1	-3	13	15.8079	1.73429	0.748374	0.00345214
694		4	-1	-3	-13	15.8079	1.04851	0.600474	0.041077
695	412	12	-6	-6	4	15.8201	1.85366	0.779941	-0.0310761
696	413	7	-1	-6	11	15.8249	0.825907	0.531444	0.0288511
697		7	-1	-6	-11	15.8249	2.04353	0.791194	-0.0147438
698	414	11	-2	-9	5	15.8588	1.50438	0.746944	-0.0516327
699		11	-2	-9	-5	15.8588	0.723134	0.485445	0.0341721
700	415	10	-3	-7	-8	15.8701	0.668659	0.487066	-0.0295615
701	416	12	-5	-7	4	15.8871	0.666969	0.470916	0.00200169
702	417	8	-1	-7	10	15.8909	1.18666	0.669003	-0.0168455
703		8	-1	-7	-10	15.8909	1.37888	0.698988	9.73E-05
704	418	11	-3	-8	6	15.9134	1.37334	0.701883	-0.00433357
705		11	-3	-8	-6	15.9134	0.959235	0.586226	0.0279367
706	419	12	-3	-9	2	15.9246	0.566658	0.408125	0.0139105
707		12	-3	-9	-2	15.9246	0.507921	0.334262	0.0686917
708	420	6	-1	-5	12	15.9753	2.07661	0.797558	-0.0103742
709		6	-1	-5	-12	15.9753	1.84825	0.777155	-0.0138946

As mentioned in the paper, the above table was calculated by an automated computer program that can automatically (and quickly) calculate the structure factors (using the principles and data similar to those in XOP) and the Darwin curves of ALL possible Bragg reflections of quartz and select the reflections satisfying specific requirements. Our program, which is freely available upon request, can be used to select all the Bragg reflections under any other specific criteria (e.g., ranges of Bragg angles, photon energies, reflectivity, bandwidths, angular acceptance, or their combinations), such that the most suitable reflections can never be missed in quartz optics design. It can also work for any other crystals if the atomic structures are known.

## Transformation of atom positions left-handed quartz to that of right-handed quartz



**Figure S1.** Mirrored position  $(x_i, x_i - y_i, z_i)$  of an atom at  $(x_i, y_i, z_i)$  with respect to the mirror plane  $A$  [parallel to the  $(1\bar{2}10)$   $\mathbf{a}$ -plane in Fig. 4(a) of the paper] in the right-handed  $\mathbf{a}_1$ - $\mathbf{a}_2$ - $\mathbf{a}_3$ - $\mathbf{c}$  hexagonal coordinate system. This operation is for transforming the left-handed quartz unit cell to the right-handed unit cell in the same right-handed hexagonal coordinate system. In the paper, this mirror operation is followed by a partial translation of  $-\mathbf{c}/3$  (which does not vary the crystal structure), so that the entire transformation is  $(x_i, y_i, z_i) \rightarrow (x_i, x_i - y_i, z_i - 1/3)$  for each atom. After this transformation, the structure factor pairs of the left- and right-handed quartz always satisfy equation (1) in the paper.